

General conditions for maximal violation of non-contextuality in discrete and continuous variables

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The contextuality of quantum mechanics, *i.e.* the measurement outcome dependence upon previously made measurements, can be shown by the violation of inequalities based on measurements of well chosen observables. An important property of such observables is that their expectation value can be expressed in terms of probabilities of obtaining two exclusive outcomes. In order to satisfy this, inequalities have been constructed using either observables with a dichotomic spectrum or using periodic functions obtained from displacement operators in phase space. Here we identify the general conditions on the spectral decomposition of observables demonstrating state independent contextuality of quantum mechanics. As a consequence, our results not only unify existing strategies for maximal violation of state independent non-contextual inequalities but also lead to new scenarii enabling such violation. Among the consequences of our results is the impossibility of having a state independent maximal violation of non-contextuality in the Peres-Mermin scenario with discrete observables of odd dimensions.

Introduction: The question of whether physical systems have intrinsic non-contextual properties is a long standing debate that was turned upside down with the advent of quantum physics. The measurement outcome dependence upon previously made measurements is at the heart of the Einstein-Podolsky-Rosen (EPR) paradox [1], that evidences the conflict between classical and quantum views of realism. The contextuality of the quantum theory, contrary to its classical analog is ensured by the Kochen-Specker theorem [2].

In a non-contextual theory, the result of a measurement $\nu(A)$ depends only on the state of the system and the observable A being measured. Additionally, measurement outcomes can depend on some (possibly hidden) variable λ describing the state of the system. If one knows λ then one can predict the outcome of any measurement: we say thus that measurement outcomes are pre-determined. This corresponds to the classical view in which every system is in a well defined state. In particular, in a non-contextual theory measurement outcomes do not depend on the compatible observables that are measured together with A .

The initial argument by Kochen-Specker to show the contextuality of quantum mechanics used a set of 117 vectors in a 3-dimensional space [2]. Since then, many attempts have been made to refine this argument and turn it into an experimentally testable property. The contextuality of quantum mechanics was proved for a particular state and a Hilbert space of dimension 4 by Peres [3]. Mermin showed that this argument could be recast to find a state independent proof of contextuality [4]. The same type of argument as Mermin's was used to derive state independent non-contextual inequalities (*i.e.*, that can be violated by any state if non-contextuality does

not hold) [5–7]. Such inequalities, obtained in the so-called Peres Mermin scenario (PMS) are particularly attractive from the experimental point of view, and have been experimentally tested with trapped ions [8], nuclear spin ensembles [9] and photons [10–12]. In addition, it has been proven that contextuality (in a state dependent formulation) is a critical resource for quantum computing [13–15].

Even though the study of contextuality was originally focused on discrete variable system, such as qubits and qudits, it is also possible to find state independent non-contextual inequalities for continuous variables in the PMS [16, 17]. In this case, one notes that the operators used to derive the inequalities have a bounded spectrum. This last property ensures that their expectation values can be expressed as the ones of dichotomic observables defined in an extended space [18]. The bounded observables used in [16, 17] can be obtained by measuring bounded functions of observables with an arbitrary spectrum, as considered in the protocols described in [16] and [17]. A similar technique led, in [19, 20], to the definition of dimension independent Bell-type inequalities [1, 21, 22], which is a particular case of non-contextual inequalities where, in addition, locality is enforced. Ruling out local realism in experiments requires to satisfy more stringent constraints that are not necessary to prove the contextuality of quantum mechanics per se. The contextuality of quantum mechanics can be proven, in principle, by measuring well chosen observables, independently of the system's particular state [23]. It is thus of interest to characterize which general properties observables must have for testing contextuality and to maximally violate experimentally testable non-contextual inequalities.

So far, the contextuality of quantum mechanics has been shown for specific observables defined by continuous or discrete variables. In addition, according to the considered case, the border between contextual and non-contextual theories varies. It is natural to seek to identify the common features of the existing results and try to formalize the general conditions quantum observables must fulfill in order to demonstrate state independent contextuality irrespectively of their dimensionality. Such understanding would potentially enable the state independent test of this essential property of quantum mechanics in any quantum system. In other words, what are the common/distinctive properties and features of non-contextual inequalities? How can one build a suitable inequality from arbitrary observables permitting the demonstration of state independent contextuality in quantum mechanics?

In this Letter we answer these questions in the PMS approach, which is, as mentioned, a particularly experimentally attractive formulation of the Kochen-Specker theorem. The PMS is shown in terms of Table I, and was originally constructed to illustrate the differences between contextual and non-contextual theories in the case of measurements of dichotomic observables that, in quantum mechanics, can be represented by the Pauli matrices. We show that the generalized version of the PMS can be obtained using complex functions (continuous or discrete) of modulus one instead of real ones. In quantum mechanics these functions are associated to unitary operations acting on a bipartite system. We will see that state independent maximal violation of non-contextual inequalities is possible iff, for each one of the considered parties, the introduced unitary operators obey specific commutation relations. These relations reduce to the known particular cases according to the chosen set-up. A consequence of our results is that in the bi-partite PMS with discrete variables, it is only possible to observe state independent maximal violation of the non-contextual bound with qudits of even dimension. Furthermore, we derive necessary and sufficient conditions the spectrum of the observable must fulfill such that it can be used for state independent maximal violation of the non-contextual bound. Our results significantly expand the possibilities of experimental state independent maximal violation of non contextual inequalities in arbitrary dimensions and provide a clear and unified framework for demonstrating the contextuality of quantum mechanics.

We start by recalling the principles of the PMS before generalizing it.

The Peres-Mermin square: Let us consider a set of nine dichotomic observables $\{A_{jk}\}$, $i, j = 1, 2, 3$, such that the observables sharing a common subscript are mutually commuting. From this set of observables, one can

TABLE I. The Peres-Mermin square for Pauli operators, $\hat{\sigma}_{x,y,z}$.

A_{jk}	$k = 1$	$k = 2$	$k = 3$
$j = 1$	$\hat{\sigma}_x \otimes 1$	$1 \otimes \hat{\sigma}_x$	$\hat{\sigma}_x \otimes \hat{\sigma}_x$
$j = 2$	$1 \otimes \hat{\sigma}_z$	$\hat{\sigma}_z \otimes 1$	$\hat{\sigma}_z \otimes \hat{\sigma}_z$
$j = 3$	$\hat{\sigma}_x \otimes \hat{\sigma}_z$	$\hat{\sigma}_z \otimes \hat{\sigma}_x$	$\hat{\sigma}_y \otimes \hat{\sigma}_y$

construct the quantity

$$\langle X \rangle = \langle A_{11}A_{12}A_{13} \rangle + \langle A_{21}A_{22}A_{23} \rangle + \langle A_{31}A_{32}A_{33} \rangle \quad (1) \\ + \langle A_{11}A_{21}A_{31} \rangle + \langle A_{12}A_{22}A_{32} \rangle - \langle A_{13}A_{23}A_{33} \rangle.$$

In a non-contextual theory, observables are described by pre-determined values -1 or 1 . One can show, by testing every possible combination of outcomes for the $\{A_{jk}\}$, that the maximum value of $\langle X \rangle$ is 4 in a non-contextual theory [5].

We now consider the case where observables $\{A_{ij}\}$ are quantum and given by Table I. One can easily check that the observables in the same row or column are compatible (commuting). Nevertheless, because the product of operators along each row and column is $\mathbb{1}$, except for the last column where it is $-\mathbb{1}$, one has that for every quantum state $\langle X \rangle_{QM} = 6$, violating the bound of 4 discussed above and thus proving that quantum mechanics is contextual in the case where dichotomic observables are measured.

The question we address now is how to generalize the PMS in order to extend the tests of the contextuality of quantum mechanics to situations where observables with fundamentally different properties from the Pauli matrices are measured. Our generalization will permit the identification of conditions that observables with an arbitrary spectrum must satisfy in order to prove contextuality.

PMS with observables with an arbitrary spectrum: Contextuality can also be tested using complex functions instead of real ones, as is the case of the previous example involving Pauli matrices. This leads to inequalities involving the (independent) real and imaginary parts of such functions. Of course, in order to test contextuality, experiments involving either the measurement of the real or the imaginary part of such functions must be carried out. Also, it is clear that since the real and imaginary parts are independent, contextuality can be independently tested for each one of these components.

Enlightening results that will be used here as a guideline were obtained by Asadian *et al.* [16], where the particular case of contextuality tests using displacements in phase space was studied. There, the authors obtain many interesting conditions and constraints for testing contextuality using displacement operators that can be well understood in the light of the general framework we obtain here.

Non-contextual inequalities involving complex functions can be derived by choosing the A_{jk} 's appearing in the PMS to be complex functions $U_{jk} = A_{jk}^R + iA_{jk}^I$, with $|A_{jk}^R|^2 + |A_{jk}^I|^2 = 1$. This leads to Table II where, in

TABLE II. The Peres-Mermin square for arbitrary operators, where U_i are arbitrary unitary operators.

A_{jk}	$k=1$	$k=2$	$k=3$
$j=1$	$\hat{U}_1^\dagger \otimes 1$	$1 \otimes \hat{U}_1^\dagger$	$\hat{U}_1 \otimes \hat{U}_1$
$j=2$	$1 \otimes \hat{U}_2^\dagger$	$\hat{U}_2^\dagger \otimes 1$	$\hat{U}_2 \otimes \hat{U}_2$
$j=3$	$\hat{U}_1 \otimes \hat{U}_2$	$\hat{U}_2 \otimes \hat{U}_1$	$\hat{U}_3 \otimes \hat{U}_3$

quantum mechanics, functions U_j become unitary operators, \hat{U}_j . For the sake of clarity, we used here a similar reasoning and notation as the one in [16], with the important difference that while Ref. [16] was restricted to the specific case of displacement operators, here we consider that operators \hat{U}_j can be arbitrary unitaries defined in a Hilbert space of arbitrary dimension. By doing so, we can identify Table I as a particular case of Table II.

By multiplying the PMS's rows and columns in Table II, we are left with an inequality involving complex functions. It can be transformed in an inequality for real functions by taking its real or imaginary parts. We will consider here its real part:

$$\langle \text{Re}(X) \rangle = \langle R_1 \rangle + \langle R_2 \rangle + \langle R_3 \rangle + \langle C_1 \rangle + \langle C_2 \rangle - \langle C_3 \rangle, \quad (2)$$

where

$$\begin{aligned} R_j &= (A_{j1}^R A_{j2}^R - A_{j1}^I A_{j2}^I) A_{j3}^R - (A_{j1}^I A_{j2}^R + A_{j1}^R A_{j2}^I) A_{j3}^I, \\ C_k &= (A_{1k}^R A_{2k}^R - A_{1k}^I A_{2k}^I) A_{3k}^R - (A_{1k}^I A_{2k}^R + A_{1k}^R A_{2k}^I) A_{3k}^I. \end{aligned} \quad (3)$$

It is now straightforward to extend the results of [16] to arbitrary complex functions of modulus one to obtain that, for non-contextual theories, $\langle \text{Re}(X) \rangle \leq 3\sqrt{3}$. A first remark made possible by the general description made so far is that if one adds the additional constraint that the real (or imaginary) part of the considered complex functions, U_j , is zero, together with the condition that the measured observables must have a dichotomic expectation value, one recovers Table I and, from (2) and (3), the non-contextual bound of 4.

We now move to the quantum description of the PMS using unitary operators. Since unitary operators are not, in general, observables, one can split them into their real and imaginary Hermitian parts, $\hat{U}_{jk} = \hat{A}_{jk}^R + i\hat{A}_{jk}^I$, which are observables. From the PMS in Table II, we can see that, in order to maximally violate the non-contextual bound, the product of the three operators in each row and column must be $\mathbb{1}$ except in the last column where it must be $-\mathbb{1}$. Also, unitaries in the same row or column must be compatible, leading to the constraints on the commutator

$[\hat{U}_1, \hat{U}_3] = 0$ or on the anti-commutator $\{\hat{U}_1, \hat{U}_3\} = 0$ and the same for \hat{U}_2 and \hat{U}_3 . These conditions cannot be verified at the same time, and the only possibility to obtain a state independent maximal violation of the non-contextual bound is to enforce $\{\hat{U}_1, \hat{U}_3\} = 0$ and $\{\hat{U}_2, \hat{U}_3\} = 0$. All the above ingredients combined lead to the following conditions for maximal violation of non-contextual inequalities based on the PMS: $\hat{U}_1 \hat{U}_2 \hat{U}_3 = \pm i\mathbb{1}$ and $\hat{U}_2 \hat{U}_1 \hat{U}_3 = \mp i\mathbb{1}$, which are equivalent to:

$$\begin{aligned} \{\hat{U}_1, \hat{U}_2\} &= 0, \\ \hat{U}_3 &= \pm i \hat{U}_2^\dagger \hat{U}_1^\dagger. \end{aligned} \quad (4)$$

From the conditions (4) we see that for state independent maximal violation of the PM inequality the operators U_1 and U_2 must be anti-commuting and that they completely determine the operator U_3 that completes the set. Thus, if the unitary operators in the PMS fulfill the commutation relations

$$\begin{aligned} \{\hat{U}_i, \hat{U}_j\} &= 2\delta_{ij} \hat{U}_i^2, \\ [\hat{U}_i, \hat{U}_j] &= \pm 2i\epsilon_{ijk} \hat{U}_k^\dagger, \end{aligned} \quad (5)$$

where ϵ_{ijk} is the Levi-Civita symbol, the expectation (2) maximally violates the non-contextual inequality with $\langle \text{Re}(X) \rangle = 6$, for all states $|\Psi\rangle$.

Conditions (4) are general, and to our knowledge, have not been established so far. Previous results showing the possibility of violation of the non-contextual inequalities are particular cases obeying these conditions. Examples are state independent contextuality using two-level systems [5] and displacement operators [16].

We now make a step further beyond the relations (4), and answer to the following question: given a unitary operator \hat{U}_1 , what are the necessary and sufficient conditions for finding two other operators \hat{U}_2 and \hat{U}_3 such that (4) is satisfied and thus lead to a maximal violation of noncontextuality inequalities derived from the Peres-Mermin square? To answer this question we have shown that a given unitary operator \hat{U}_1 , acting on a Hilbert space \mathcal{H} , admits an anti-commuting partner if and only if for each eigenvalue λ of \hat{U}_1 , we find a corresponding eigenvalue $-\lambda$ whose eigenspace has the same dimension K as the one of λ . Once we have found an operator that fulfills this statement we can express it in some basis as a direct sum:

$$\hat{U}_1 = \bigoplus_{i=1}^N \lambda_i \hat{\sigma}_z^{(i)}, \quad (6)$$

where $\pm\lambda_i$ are the eigenvalues of \hat{U}_1 , $\hat{\sigma}_z^{(i)} = \bigoplus_{j=1}^{K_i} \hat{\sigma}_z$ is a direct sum of Pauli operators acting on the eigenspace associated to the eigenvalue $\pm\lambda_i$ with degeneracy K_i , and N is an arbitrary, possibly infinite, integer value that is smaller than the Hilbert space dimension. In the particular case of a nondegenerate spectrum $\hat{\sigma}_z^{(i)} = \hat{\sigma}_z$ acts on

a two dimensional subspace. Anti-commuting partners to \hat{U}_1 are given by:

$$\hat{U}_2 = \bigoplus_{i=1}^N \lambda'_i \hat{\sigma}_x^{(i)}, \quad \hat{U}_3 = \pm \bigoplus_{i=1}^N (\lambda_i \lambda'_i)^* \hat{\sigma}_y^{(i)}, \quad (7)$$

where $\hat{\sigma}_x^{(i)} = \bigoplus_{j=1}^{K_i} \hat{\sigma}_x$, $\hat{\sigma}_y^{(i)} = \bigoplus_{j=1}^{K_i} \hat{\sigma}_y$ and the expression of \hat{U}_3 follows directly from Eq. (4). Diagonalization of Eq. (11) yields for \hat{U}_2 and \hat{U}_3 the same form as in (6). This shows that maximal state-independent contextuality in the PMS is a very peculiar property related to spectrum of operators whose spectral decomposition, continuous or discrete, can be written in terms of finite or infinite direct sums of Pauli matrices weighted by complex numbers of modulus one.

We will now study some examples of operators satisfying the presented conditions and show how the already used ones are special cases of the general form (6). One can directly see that the case $N = 1$ and $\lambda_1 = 0$ corresponds to the case described in Table I.

Finite N: The decomposition (6) (and the ones equivalent to it up to an unitary transformation) imposes a parity condition on the spectrum of operators enabling a maximal violation of the non-contextual inequalities in the PMS for finite N . Thus, state independent maximal violation of contextuality in a Peres-Mermin scenario is only possible in a Hilbert space of even dimension and formed by two parties which are themselves of even dimension as well. In [16], the authors reached a similar conclusion for the case of discrete displacements in phase space. Thanks to the generality of the conditions obtained here, we can analyze in detail a scenario where a naturally discrete system is considered, introducing new operators enabling contextuality tests for qudits.

Considering the case of a pair of spin S particles, contextuality in the PMS can be demonstrated by using the following rotation operators:

$$\hat{R}_1 = e^{i\hat{S}_x t_1}, \quad \hat{R}_2 = e^{i\hat{S}_y t_2}, \quad \hat{R}_3 = e^{i\hat{S}_z t_3}, \quad (8)$$

where \hat{S}_x , \hat{S}_y and \hat{S}_z are the three components of a spin $\hat{\vec{S}}$, the 3 generators of SU(2) in $d = 2S + 1$ dimensional Hilbert space. In order to build a PMS, one must choose t_1 , t_2 and t_3 such that R_1 , R_2 and R_3 verify (6). We have $(S_z)_{ij} = (S + 1 - b)\delta_{i,j}$, and the eigenvalues of R_3 are $\exp(i(S + 1 - b)t_1)$ for $j = 1, 2, \dots, d$. They will fulfill the condition (6) only if $t_3 = \pi$. Since S_x and S_y are unitarily equivalents to S_z , condition (6) is verified only if $t_1 = t_2 = \pi$ as well. In this case, we can check that R_1 , R_2 and R_3 satisfy (4), showing that it is possible to construct a similar structure as the PMS using the rotation operators of half-integer spins, generalizing Table I.

We now study the case of observables for which $N \rightarrow \infty$. A first interesting and illustrating particular case is the one of $N \rightarrow \infty$ and $\lambda_n = 0$. In this

case, (6) reduces to the parity operator: the observable $\bigoplus_{n=1}^N \hat{\sigma}_z^{(n)}$ has a binary spectrum and by choosing $\hat{\sigma}_z^{(n)} = |2n\rangle\langle 2n| - |2n+1\rangle\langle 2n+1|$, for instance, we have $\hat{U}_1 = \bigoplus_{n=1}^N \hat{\sigma}_z^{(n)} = (-1)^{\hat{n}}$, with $\hat{n}|n\rangle = n|n\rangle$. It is easy to show that for $\hat{U}_2 = \bigoplus_{n=1}^N |2n\rangle\langle 2n+1| + |2n+1\rangle\langle 2n|$ and $\hat{U}_3 = \bigoplus_{n=1}^N i(|2n\rangle\langle 2n+1| - |2n+1\rangle\langle 2n|)$ the condition (4) is satisfied. These kind of pseudospin operators were also used to show that the EPR state can lead to a maximal violation of nonlocality in terms of the CHSH inequality [27].

Our result can also be described in terms of continuous variables (CV) using an infinite continuous direct sum. To further develop this we start by describing a previously studied case and generalize it. It has been shown in [16] that using displacement operators in phase space $\hat{U}_1 = \mathcal{D}(\alpha_1) = e^{\alpha_1 \hat{a}^\dagger - \alpha_1^* \hat{a}}$, we can always find other displacement operators $\mathcal{D}(\alpha_2)$ and $\mathcal{D}(\alpha_3)$ that satisfy the relations (4) and thus maximally violates the contextual bound for any state described by CV. The condition for this is α_2 and α_3 such that $\text{Im}(\alpha_i \alpha_j^*) = \pm\pi/2$ and $\alpha_1 + \alpha_2 + \alpha_3 = 0$. A particularly suitable way to see that this case can be described by the form (6) is using the modular variable basis and the formalism developed in [26]. Within this formalism, one can show that

$$\mathcal{D}(\alpha_1) = e^{i2\pi\hat{x}/\ell} = \int_{-\ell/4}^{\ell/4} d\bar{x} \int_{-\pi/\ell}^{\pi/\ell} d\bar{p} e^{i2\pi\bar{x}/\ell} \hat{\sigma}_z(\bar{x}, \bar{p}), \quad (9)$$

where $\hat{\sigma}_z(\bar{x}, \bar{p}) = |\bar{x}, \bar{p}\rangle\langle \bar{x}, \bar{p}| - |\bar{x} + \ell/2, \bar{p}\rangle\langle \bar{x} + \ell/2, \bar{p}|$ is a $\hat{\sigma}_z$ Pauli-like matrix in the two dimensional subspace defined by $|\bar{x}, \bar{p}\rangle$ and $|\bar{x} + \ell/2, \bar{p}\rangle$. Variables \bar{x} , \bar{p} are bounded, such that $\bar{x} \in [-\ell/2, \ell/2[$ and $\bar{p} \in [-\pi/\ell, \pi/\ell[$ (see [26] for more details). We see that (9) has the form of (6) where we used a continuous sum instead of a discrete one due to the nature of the chosen basis. In this framework, the eigenvalues of $\hat{U}_1 = \mathcal{D}(\alpha_1)$ are given by $\pm e^{i2\pi\bar{x}/\ell}$. From (9), one can directly derive $\mathcal{D}(\alpha_2) = e^{-i\hat{p}\ell/2} = \int_{-\ell/4}^{\ell/4} d\bar{x} \int_{-\ell/4}^{\ell/4} d\bar{p} e^{-i\bar{p}\ell/2} \hat{\sigma}_x(\bar{x}, \bar{p})$ and $\mathcal{D}(\alpha_3) = i\mathcal{D}(\alpha_2)^\dagger \mathcal{D}(\alpha_1)^\dagger = \int_{-\ell/4}^{\ell/4} d\bar{x} \int_{-\ell/4}^{\ell/4} d\bar{p} e^{-i\bar{p}\ell/2 + 2\pi i\bar{x}/\ell} \hat{\sigma}_x(\bar{x}, \bar{p})$ from the commutation relations between $\hat{\sigma}_x(\bar{x}, \bar{p})$ and $\hat{\sigma}_y(\bar{x}, \bar{p})$ (see [26]), defined as $\hat{\sigma}_x(\bar{x}, \bar{p}) = |\bar{x}, \bar{p}\rangle\langle \bar{x} + \ell/2, \bar{p}| + |\bar{x} + \ell/2, \bar{p}\rangle\langle \bar{x}, \bar{p}|$ and $\hat{\sigma}_y(\bar{x}, \bar{p}) = i(|\bar{x}, \bar{p}\rangle\langle \bar{x} + \ell/2, \bar{p}| - |\bar{x} + \ell/2, \bar{p}\rangle\langle \bar{x}, \bar{p}|)$.

The continuum of eigenvalues $\pm e^{i2\pi\bar{x}/\ell}$ in (9) are a specific case, and using the general form $\pm e^{i\lambda(\bar{x}, \bar{p})}$ would equally well satisfy the symmetry conditions identified for \hat{U}_1 using operators with a spectrum different from the one of the displacement operators. For those who are less familiar with the (complete) modular variable basis, we stress that the general structure of (6) does not depend on the basis, and operators as $\hat{U}_1 = \int_0^\infty dx e^{if(x)} \hat{\sigma}_z(x)$, with $\sigma_z(x) = |x\rangle\langle x| - |-x\rangle\langle -x|$ are, of course, equally suitable for maximal violation of non-contextual inequalities.

Conclusion: We derived general conditions for a operator to maximally violate non-contextual inequalities in the Peres-Mermin scenario irrespectively of the dimension of the system used to test it. A consequence of our results is that it is not possible to maximally violate such inequalities for any state using bipartite systems where one of the systems is in an odd dimensional Hilbert space. Nevertheless, we show how contextuality can be demonstrated using systems of arbitrarily high dimensional subsystems and in continuous variables. In both the discrete and continuous case we find a characterization in terms of their spectrum of observables that can be used to maximally violate the non-contextual bound in the Peres-Mermin inequality. This characterization allow us to find a natural decomposition of the observables in terms of Pauli matrices. Perspectives of our results are implementation of contextuality tests using a wide range of observables both in the discrete and continuous regime and relating the obtained conditions to the possibility of implementing quantum information protocols with continuous variables.

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SUPPLEMENTARY MATERIAL

In this Supplementary Material we provide detailed derivation of result (6) presented in the main part of the present manuscript, in the finite dimensional case.

PROOF OF RESULT (6)

Let \hat{U} be an unitary operator acting on the Hilbert space \mathcal{H} . We want to prove that there is an unitary operator that anti-commutes with \hat{U} if and only if for each eigenvalue λ of \hat{U} , $-\lambda$ is also an eigenvalue and the eigenspaces have the same dimension.

Proof: To prove the above statement we assume first that \hat{U} fulfills the above condition on the spectrum and proof that it admits an anti-commuting partner. We restrict ourselves here to a proof in the finite dimensional case. Let's define the set of eigenvalues of \hat{U} as $\{\lambda_1, \dots, \lambda_k, -\lambda_1, \dots, -\lambda_k\}$, and the set of eigenvectors associated to each of the eigenvalues $\pm\lambda_i$ as $\{|e_{i,j}^\pm\rangle\}$, with possible degeneracy $j \in \{1, \dots, K_i\}$. Since \hat{U} is a unitary operator, we know that the set of eigenvectors $\{|e_{i,j}^\pm\rangle\}$ represents an orthonormal basis of the Hilbert space. Further on, we define an operator \hat{U}' through: $\hat{U}'|e_{i,j}^\pm\rangle = \lambda'_i|e_{i,j}^\mp\rangle$, where λ'_i are arbitrary complex numbers with absolute value 1, which maps an orthonormal basis to another orthonormal basis thus providing a uni-

tary operator. A simple calculation yields:

$$\begin{aligned} (\hat{U}\hat{U}' + \hat{U}'\hat{U})|e_{i,j}^\pm\rangle &= \lambda'_i\hat{U}|e_{i,j}^\mp\rangle \pm \lambda_i\hat{U}'|e_{i,j}^\pm\rangle \\ &= \mp\lambda_i\lambda'_i|e_{i,j}^\mp\rangle \pm \lambda_i\lambda'_i|e_{i,j}^\mp\rangle = 0. \end{aligned} \quad (10)$$

showing that \hat{U} and \hat{U}' are anti-commuting. Hence, we have found an anti-commuting partner to \hat{U} defined through the condition $\hat{U}'|e_{i,j}^\pm\rangle = |e_{i,j}^\mp\rangle$, leading to the expression:

$$\hat{U}' = \bigoplus_{i=1}^N \lambda'_i \sigma_x^{(i)}, \quad (11)$$

where $\sigma_x^{(i)} = \bigoplus_{j=1}^{K_i} \sigma_x$. Diagonalization of Eq. (11) yields for \hat{U}_2 the same form as in (6).

To prove the converse statement let's assume that we have two unitary operators \hat{U} and \hat{U}' satisfying $\{\hat{U}, \hat{U}'\} = 0$. We denote by λ an eigenvalue of \hat{U} with the corresponding eigenvectors $|\{e_i\}\rangle$, where $i = 1 \dots K$. Using the anti-commutation relation we can prove that $\hat{U}'|e_i\rangle$ is an eigenvector of \hat{U} with eigenvalue $-\lambda$:

$$(\hat{U}\hat{U}' + \hat{U}'\hat{U})|e_i\rangle = \hat{U}\hat{U}'|e_i\rangle + \hat{U}'\lambda|e_i\rangle \quad (12)$$

$$\Rightarrow \hat{U}\hat{U}'|e_i\rangle = -\lambda\hat{U}'|e_i\rangle. \quad (13)$$

Since $\{|e_i\rangle\}$ is an orthonormal set and \hat{U}' is a unitary operator, $\{\hat{U}'|e_i\rangle\}$ is also an orthonormal set, which proves that $-\lambda$ is an eigenvalue of \hat{U} of dimension larger or equal than K . The same reasoning applied to the set of eigenvectors of \hat{U} with eigenvalue $-\lambda$ to show that the dimension of the eigenspace associated to λ is higher or equal than the dimension of the eigenspace associated to $-\lambda$ and thus equal.

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